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Variable-Step Truncation Error Estimates for Runge–Kutta Methods of Order 4 or Less*

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One of the primary drawbacks in the use of Runge–Kutta for the solution of the initial-value problem for ordinary differential equations is the high price one must pay in computer time in order to gain an accurate estimate of the local truncation error. A very common practice with Runge–Kutta is to do the calculations with a given step-size h and simultaneously do the calculations with step-size $2h$. A combination of the two answers thus produced is then used to control step-size.

In this paper we derive and test some estimates for variable step-size Runge–Kutta which are accurate and which do not require any other function evaluations than those normally used by Runge–Kutta. In addition, one method for using these estimates is presented along with numerical results.

1. INTRODUCTION

One method of controlling the step-size for Runge–Kutta methods for ordinary differential equations is to calculate an estimate of the local truncation error. Very accurate estimates for this error have been obtained by Morel [4] and Kuntzmann [3]. These methods are compared with other estimators by Shampine and Watts [6]. However, these estimates are based on a fixed step-size procedure (or at least where the step-size has remained unchanged for several steps) and are not well known despite their accuracy. In this paper estimates are derived which are applicable in the variable step-size case for Runge–Kutta (and other one-step methods) of order 4 (globally) or less. The estimates are accurate but inconvenient for programming. Their use will surely be limited to library codes for solving differential equations and to large problems where a fair amount of coding can be tolerated.

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2. Definitions

In order to approximate the solution of the initial-value problem,

$$\begin{aligned} y'(x) &= f(x, y(x)), \\ y(a) &= A, \end{aligned} \tag{2.1}$$

one often uses a scheme of the form,

$$\begin{aligned} y_{n+1} &= y_n + h_n \Phi(x_n, y_n, h_n) \\ y_0 &= A, \end{aligned} \tag{2.2}$$

where $x_{n+1} = x_n + h_n$, $x_0 = a$, $h_n > 0$ but variable. Such schemes are called one-step methods, the classical Runge–Kutta of order 4 being an example. If the solution y_n of the approximating problem (2.2) could be found exactly (i.e., no round-off error), then number y_n would still, in general, differ from $y(x_n)$, the solution of (2.1). The difference $y(x_n) - y_n$ will be referred to as the total error at x_n due to truncation. To define the local truncation error at x_n (actually from x_n to x_{n+1}) let us assume that we have the exact solution y_n, of (2.2) and define $Z_n(x)$ by

$$\begin{aligned} Z_n'(x) &= f(x, Z_n(x)), \\ Z(x_n) &= y_n . \end{aligned} \tag{2.3}$$

Thus, $Z_n(x)$ is an integral curve of the differential equation associated with (2.1) which passes through the point (x_n, y_n). The local truncation error in going from x_n to x_{n+1}, denoted by τ_n, is defined by

$$\tau_n = Z_n(x_{n+1}) - y_{n+1} . \tag{2.4}$$

Let us define $\Omega(j, i)$ by

$$\Omega(j, i) = Z_j(x_{j+i}) - y_{j+i} , \tag{2.5}$$

and note that $\Omega(n, 1) = \tau_n$. However, $\Omega(n, -1) = Z_n(x_{n-1}) - y_{n-1}$; whereas $\tau_{n-1} = Z_{n-1}(x_n) - y_n$. If the integral curves Z_n and Z_{n-1} (see Fig. 1) remained the same distance apart between x_{n-1} and x_n, then we would have $\tau_n = -\Omega(n, -1)$. This "nonparallel" property of the integral curves causes a reasonable amount of difficulty in the derivations of the error estimate. One should not, however, lose sight of the fact that the estimates would be very nearly as good if we ignored this point, as we prove below.

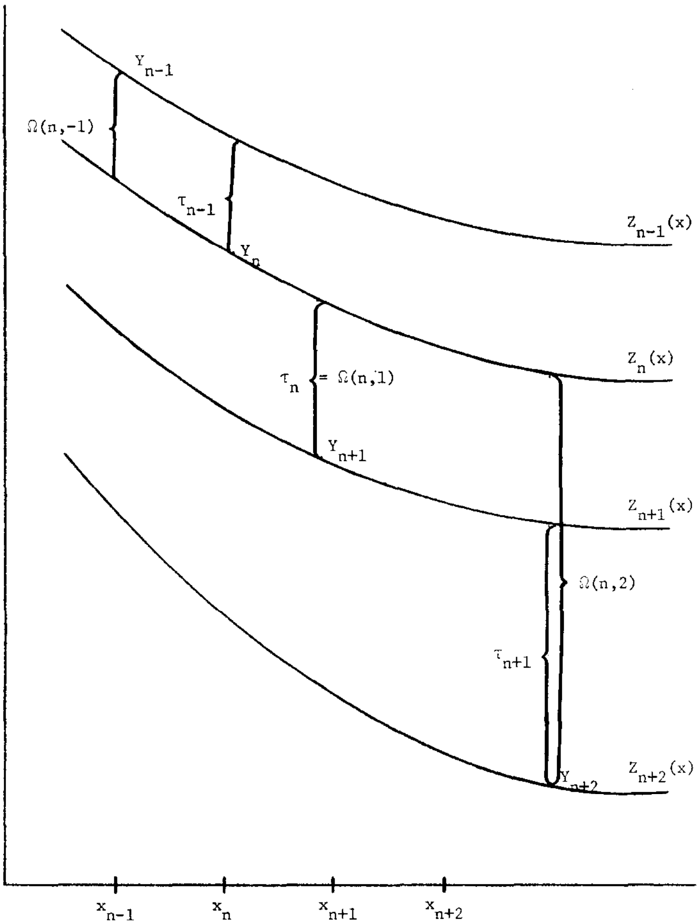

FIGURE 1

3. ESTIMATES FOR $\Omega(j, i)$

From (2.5) one has

$$\begin{aligned}\Omega(n, -1) &= Z_n(x_{n-1}) - y_{n-1} \\ &= -[Z_{n-1}(x_n - h_{n-1}) - Z_n(x_n - h_{n-1})] \\ &= -\Big\{[Z_{n-1}(x_n) - Z_n(x_n)] - h_{n-1}[Z'_{n-1}(x_n) - Z_n'(x_n)] \\ &\quad + \frac{h_{n-1}^2}{2}[Z''_{n-1}(x_n) - Z''_n(x_n)] - \frac{h_{n-1}^3}{6}[Z'''_{n-1}(x_n) - Z'''_n(x_n)] + \cdots\Big\}. \end{aligned} \tag{3.1}$$

We need estimates for the first few terms of (3.1):

1st term

$$Z_{n-1}(x_n) - Z_n(x_n) = Z_{n-1}(x_n) - y_n = \tau_n .$$

2nd term

$$\begin{aligned} h_{n-1}[Z'_{n-1}(x_n) - Z_n'(x_n)] &= h_{n-1}[f(x_n , Z_{n-1}(x_n)) - f(x_n , Z_n(x_n))] \\ &= h_{n-1}[f(x_n , \tau_{n-1} + y_n) - f(x_n , y_n)] \\ &= h_{n-1}\tau_{n-1} f_y(x_n , y_n) + O(h_{n-1}\tau_{n-1}^2). \end{aligned}$$

3rd term

Now

$$Z_j''(x) = f'(x, Z_j(x)) = f_x(x, Z_j(x)) + f_y(x, Z_j(x)) f(x, Z_j(x)).$$

Hence, the 3rd term becomes

$$\begin{aligned} &\tfrac{1}{2} h_{n-1}^2\{[f_x(x_n , \tau_{n-1} + y_n) - f_x(x_n , y_n)] \\ &\qquad + [f_y(x_n , \tau_{n-1} + y_n) f(x_n , \tau_{n-1} + y_n) - f_y(x_n , y_n) f(x_n , y_n)]\} \\ &= \tfrac{1}{2} h_{n-1}^2\{\tau_{n-1} f_{xy}(x_n , y_n) + O(\tau_{n-1}^2) + f_{yy}(x_n , y_n) f(x_n , y_n)\, \tau_{n-1} \\ &\qquad + f_y^2(x_n , y_n)\, \tau_{n-1} + f_{yy}(x_n , y_n) f_y(x_n , y_n)\, \tau_{n-1}^2\} \\ &= O(h_{n-1}^2\tau_{n-1}) + O(h^2\tau_{n-1}^2). \end{aligned}$$

We may continue this process by expressing the higher order derivatives of Z_j in terms of the total derivatives of f, but the resultant terms will be bounded by $O(h^p\tau_{n-1}) + O(h^p\tau_{n-1}^2)$ where p is the order of the derivative of Z_j.

Using these expressions in (3.1) one has

$$\Omega(n, -1) = -(1 - h_{n-1} f_y(x_n , y_n))\, \tau_{n-1} + O(h_{n-1}\tau_{n-1}^2) + O(h_{r-1}^2\tau_{n-1}). \tag{3.2}$$

The essence of the derivation of $\Omega(n, -2)$ is

$$\begin{aligned} \Omega(n, -2) &= [Z_n(x_{n-1} - h_{n-2}) - y_{n-1}] + [y_{n-1} - Z_{n-2}(x_{n-1} - h_{n-2})] \\ &= [Z_n(x_{n-1}) - y_{n-1}] - [Z_{n-2}(x_{n-1}) - y_{n-1}] \\ &\quad - h_{n-2}[Z_n'(x_{n-1}) - Z'_{n-2}(x_{n-1})] \\ &\quad + \tfrac{1}{2} h_{n-2}^2[Z_n''(x_{n-1}) - Z''_{n-2}(x_{n-1})] + \cdots \\ &= \Omega(n, -1) - \tau_{n-2} \\ &\quad - h_{n-2}[f(x_{n-1} , y_{n-1} + \Omega(n, -1)) - f(x_{n-1} , \tau_{n-2} + y_{n-1})] + \cdots \\ &= -(1 - h_{n-1} f_y(x_n , y_n))\, \tau_{n-1} - \tau_{n-2} \\ &\quad - h_{n-2}[f_y(x_{n-1} , y_{n-1})\, \Omega(n, -1) - f_y(x_{n-1} , y_{n-1})\, \tau_{n-1}] + \cdots \\ &= -[1 - h_{n-1} f_y(x_n , y_n) - h_{n-2} f_y(x_{n-1} , y_{n-1}) \\ &\quad + h_{n-1}h_{n-2} f_y(x_{n-1} , y_{n-1}) f_y(x_n , y_n)]\, \tau_{n-1} \\ &\quad - (1 - h_{n-2} f_y(x_{n-1} , y_{n-1}))\, \tau_{n-2} + \cdots . \end{aligned} \tag{3.3}$$

From the definition of $\Omega(j, i)$ and from (3.2) and (3.3) one has

$$
\begin{aligned}
z_n(x_n) &= y_n , \\
Z_n(x_{n+1}) &= y_{n+1} + \tau_n , \\
Z_n(x_{n-1}) &= y_{n-1} - (1 - h_{n-1} f_y(x_n , y_n))\, \tau_{n-1} , \\
Z_n(x_{n-2}) &= y_{n-2} - (1 - h_{n-2} f_y(x_{n-1} , y_{n-1}))\, \tau_{n-2} \\
&\quad - [1 - h_{n-1} f_y(x_n , y_n) - h_{n-2} f_y(x_{n-1} , y_{n-1})]\, \tau_{n-1} ,
\end{aligned} \tag{3.4}
$$

where we have neglected terms of the order $O(h^2\tau_j)$ and $O(\tau_j^2)$. We also have

$$
\begin{aligned}
Z_n'(x_n) &= f(x_n , Z_n(x_n)) = f(x_n , y_n), \\
Z_n'(x_{n+1}) &= f(x_{n+1} , \tau_n + y_{n+1}) = f(x_{n+1} , y_{n+1}) + f_y(x_{n+1} , y_{n+1})\, \tau_n , \\
Z_n'(x_{n-1}) &= f(x_{n-1} , y_{n-1}) - (1 - h_{n-1} f_y(x_n , y_n)) f_y(x_{n-1} , y_{n-1})\, \tau_{n-1} , \\
Z_n'(x_{n-2}) &= f(x_{n-2} , y_{n-2}) - (1 - h_{n-2} f_y(x_{n-1} , y_{n-1})) f_y(x_{n-2} , y_{n-2})\, \tau_{n-2} \\
&\quad - [1 - h_{n-1} f_y(x_n , y_n) - h_{n-2} f_y(x_{n-1} , y_{n-1})] f_y(x_{n-2} , y_{n-2})\, \tau_{n-1} .
\end{aligned} \tag{3.5}
$$

4. Polynomial Relations

For a polynomial, P_{2m-2}, of degree $2m - 2$ there exists a relation between the values of P_{2m-2} and its first derivative at the m distinct abscissas $\alpha_1 ,..., \alpha_m$. If $m = 2$ and $\alpha_2 - \alpha_1 = h$, the relation is

$$2P_2(\alpha_1) + hP_2'(\alpha_1) = 2P_2(\alpha_2) - hP_2'(\alpha_2).$$

If we are given a function $g(\alpha)$ which is differentiable, how much error do we incur by using the polynomial relation for g? For $m = 2$ we are asking what $E(\alpha, g)$ is in the relation

$$2g(\alpha_1) + hg'(\alpha_1) = 2g(\alpha_2) - hg'(\alpha_2) + E(\alpha, g).$$

Huddleston answers this question for the nonevenly spaced step-size case in [1]. The relation is given by

$$\sum_{i=1}^{m} \left\{ \prod_{\substack{j=1 \\ j \neq i}}^{m-1} \left(\frac{\alpha_m - \alpha_j}{\alpha_i - \alpha_j} \right)^2 \left[g'(\alpha_i) - \left(\sum_{\substack{j=1 \\ j \neq i}}^{m} \frac{2}{\alpha_i - \alpha_j} \right) g(\alpha_i) \right] \right\} = - E(\alpha_m , g), \tag{4.1}$$

where

$$E(\alpha_m , g) = - \frac{\prod_{j=1}^{m-1} (\alpha_n - \alpha_j)^2 \, g^{(2m-1)}(\xi)}{2(2m - 1)! \sum_{j=1}^{m-1} \left(\frac{1}{\alpha_m - \alpha_j} \right)}, \tag{4.2}$$

ξ being an element of the smallest interval containing $\alpha_1, \alpha_2, \ldots, \alpha_m$. Letting $m = 4$, $\alpha_i = x_{n-3+i}$, $i = 1, \ldots, 4$, $g = Z_n$, $h = x_{n+1} - x_n$, $x_{n-1} = x_n - d_1 h$, and $x_{n-2} = x_n - d_2 h$, the relation (4.1) becomes

$$\begin{aligned}
&\left[hZ_n'(x_{n+1}) - 2\left(\frac{1}{1+d_2} + \frac{1}{1+d_1} + 1\right) Z_n(x_{n+1})\right] \\
&\quad + \left(\frac{1+d_2}{d_2}\right)^2 \left(\frac{1+d_1}{d_1}\right)^2 \left[hZ_n'(x_n) - 2\left(\frac{1}{d_2} + \frac{1}{d_1} - 1\right) Z_n(x_n)\right] \\
&\quad + \left(\frac{1+d_2}{d_2-d_1}\right)^2 \left(\frac{1}{d_1}\right)^2 \\
&\quad \times \left[hZ_n'(x_{n-1}) - 2\left(\frac{1}{d_2-d_1} - \frac{1}{d_1} - \frac{1}{1+d_1}\right) Z_n(x_{n-1})\right] \\
&\quad + \left(\frac{1+d_1}{d_1-d_2}\right)^2 \left(\frac{1}{d_2}\right)^2 \\
&\quad \times \left[hZ_n'(x_{n-2}) - 2\left(\frac{1}{d_1-d_2} - \frac{1}{d_2} - \frac{1}{1+d_2}\right) Z_n(x_{n-2})\right] \\
&= -E,
\end{aligned} \tag{4.3}$$

where $-E$ is of the order H^7 with $H = \max\{h, d_1 h, x_{n-1} - x_{n-2}\}$. In the following we shall designate the order of E to be $O(h^7)$, which is sufficiently accurate for our purpose.

Substituting the relations (3.4) and (3.5) into (4.3) and ignoring terms like $O(h^2\tau_j)$ we have,[1]

$$\begin{aligned}
&\Bigg\{\left(\frac{1+d_1}{d_1-d_2}\right)^2 \left(\frac{1}{d_2}\right)^2 \Bigg[2\left(\frac{1}{d_1-d_2} - \frac{1}{d_2} - \frac{1}{1+d_2}\right) \\
&\qquad \times \left(1 - (d_2-d_1)\, hf_y(x_{n-1}, y_{n-1})\right) - hf_y(x_{n-2}, y_{n-2})\Bigg]\Bigg\}\, \tau_{n-2} \\
&\qquad + \Bigg\{\left(\frac{1+d_2}{d_2-d_1}\right)^2 \left(\frac{1}{d_1}\right)^2 \Bigg[2\left(\frac{1}{d_2-d_1} - \frac{1}{d_1} - \frac{1}{1+d_1}\right) \\
&\qquad \times \left(1 - d_1 hf_y(x_n, y_n)\right) - hf_y(x_{n-1}, y_{n-1})\Bigg] \\
&\qquad + \left(\frac{1+d_1}{d_1-d_2}\right)^2 \left(\frac{1}{d_2}\right)^2 \Bigg[2\left(\frac{1}{d_1-d_2} - \frac{1}{d_2} - \frac{1}{1+d_2}\right) \\
&\qquad \times \left(1 - d_1 hf_y(x_n, y_n) - (d_2-d_1)\, hf_y(x_{n-1}, y_{n-1})\right) \\
&\qquad - hf_y(x_{n-1}, y_{n-2})\Bigg]\Bigg\}\, \tau_{n-1} \\
&\qquad + \left\{hf_y(x_{n+1}, y_{n+1}) - 2\left(\frac{1}{1+d_2} + \frac{1}{1+d_1} + 1\right)\right\} \tau_n
\end{aligned}$$

[1] Note that h_n is now h, h_{n-1} is $d_1 h$, and h_{n-2} is $(d_2 - d_1)h$.

$$
\begin{aligned}
&= \left(\frac{1+d_1}{d_1-d_2}\right)^2 \left(\frac{1}{d_2}\right)^2 \\
&\quad \times \left[2\left(\frac{1}{d_1-d_2} - \frac{1}{d_2} - \frac{1}{1+d_2}\right) y_{n-2} - hf(x_{n-2}, y_{n-2})\right] \\
&\quad + \left(\frac{1+d_2}{d_2-d_1}\right)^2 \left(\frac{1}{d_1}\right)^2 \\
&\quad \times \left[2\left(\frac{1}{d_2-d_1} - \frac{1}{d_1} - \frac{1}{1+d_1}\right) y_{n-1} - hf(x_{n-1}, y_{n-1})\right] \\
&\quad + \left(\frac{1+d_2}{d_2}\right)^2 \left(\frac{1+d_1}{d_1}\right)^2 \left[2\left(\frac{1}{d_2} + \frac{1}{d_1} - 1\right) y_n - hf(x_n, y_n)\right] \\
&\quad + \left[2\left(\frac{1}{1+d_2} + \frac{1}{1+d_1} + 1\right) y_{n+1} - hf(x_{n+1}, y_{n+1})\right] + O(h^7).
\end{aligned} \tag{4.4}
$$

Equation (4.4) is the error estimate which we were seeking. However, there are two drawbacks to (4.4): (i) its use requires knowledge of f_y at several points; and (ii) it gives a linear combination of τ_{n-2}, τ_{n-1}, and τ_n rather than explicit estimates of the truncation error at one step. Several methods of using (4.4) suggest themselves. The requirement that f_y be known can be overcome by using $O(h)$ approximations to f_y without lowering the h^7 order of estimation. The linear combination property is more serious.

5. Estimates for Numerical Results

Let us apply the estimate (4.4) to a Runge–Kutta method of order 4 [locally $O(h^5)$], and strive to have the estimate accurate to $O(h^6)$. Then we may dispose of all terms which are like $O(h\tau)$. Following the lead of Shampine [5, pp. 6 and 25] we say that the local error τ is sufficiently smooth so that

$$\tau_{n-i} = \tau + O(h\tau).$$

With these assumptions, estimate (4.4) becomes

$$
\begin{aligned}
&\Bigg\{2\left(\frac{1+d_1}{d_1-d_2}\right)^2 \left(\frac{1}{d_2}\right)^2 \left(\frac{1}{d_1-d_2} - \frac{1}{d_2} - \frac{1}{1+d_2}\right) \\
&\quad + \left(\frac{1+d_2}{d_2-d_1}\right)^2 \left(\frac{1}{d_1}\right)^2 \left(\frac{1}{d_2-d_1} - \frac{1}{d_1} - \frac{1}{1+d_1}\right) \\
&\quad - \left(\frac{1}{1+d_2} + \frac{1}{1+d_1} + 1\right)\Bigg\}\, \tau
\end{aligned}
$$

$$
\begin{aligned}
= - \Big\{ & \left(\frac{1}{1 + d_2} + \frac{1}{1 + d_1} + 1\right) y_{n+1} \\
& + \left(\frac{1 + d_2}{d_2}\right)^2 \left(\frac{1 + d_1}{d_1}\right)^2 \left(\frac{1}{d_2} + \frac{1}{d_1} - 1\right) y_n \\
& + \left(\frac{1 + d_2}{d_2 - d_1}\right)^2 \left(\frac{1}{d_1}\right)^2 \left(\frac{1}{d_2 - d_1} - \frac{1}{d_1} - \frac{1}{1 + d_1}\right) y_{n-1} \\
& + \left(\frac{1 + d_1}{d_1 - d_2}\right)^2 \left(\frac{1}{d_2}\right)^2 \left(\frac{1}{d_1 - d_2} - \frac{1}{d_2} - \frac{1}{1 + d_2}\right) y_{n-2} \Big\} \\
& + \frac{h}{2} \Big\{ f_{n+1} + \left(\frac{1 + d_2}{d_2}\right)^2 \left(\frac{1 + d_1}{d_1}\right)^2 f_n + \left(\frac{1 + d_2}{d_2 - d_1}\right)^2 \left(\frac{1}{d_1}\right)^2 f_{n-1} \\
& + \left(\frac{1 + d_1}{d_1 - d_2}\right)^2 \left(\frac{1}{d_2}\right)^2 f_{n-2} \Big\} .
\end{aligned}
$$

This is the estimate we shall use for numerical testing.

6. Numerical Results

Numerical results are given here for the following three initial value problems:

$$
\begin{aligned}
& y' = -2\,x\,y^2, && \text{Solution: } y(x) = [1 + x^2]^{-1}, \\
& y(0) = 1, && \\
& \text{Integral curve through } (a, b): && \\
& \qquad Z(x) = b[1 + (x^2 - a^2)\, b]^{-1}. &&
\end{aligned}
\tag{6.1}
$$

$$
\begin{aligned}
& y' = 5y + 20\pi e^{5x} \cos 20\pi x, && \text{Solution: } y(x) = e^{5x} \sin 20\pi x, \\
& y(0) = 0, && \\
& \text{Integral curve through } (a, b): && \\
& \qquad Z(x) = b e^{5(x-a)} + e^{5x}[\sin 20\pi x - \sin 20\pi a]. &&
\end{aligned}
\tag{6.2}
$$

$$
\begin{aligned}
& y' = 100(y - x) && \text{Solution: } y(x) = x + \frac{1}{100} \\
& y(0) = \frac{1}{100} && \\
& \text{Integral curve through } (a, b): && \\
& \qquad Z(x) = x + \frac{1}{100} + e^{100(x-a)} \left(b - a - \frac{1}{100}\right) . &&
\end{aligned}
\tag{6.3}
$$

The routine was started with a step-size of 0.001. Each time the routine was run maximum, $T_{\max}$, and minimum, $T_{\min}$, values were set for the local truncation error τ_{n-1}. The step-size was halved if the maximum was exceeded and increased by a factor of 1.25 if τ_{n-1} fell below the minimum. The question with which we are concerned is whether (5.1) yields a good estimate of the true local truncation error. Hence, for each step we have also calculated the true local truncation error as defined by (2.4). All of the calculations presented here are for $T_{\max} = 5 \times 10^{-8}$ and $T_{\min} = 5 \times 10^{-10}$. Many other values were tested with similar results.

TABLE I[a]

x	y (calculated solution)	Relative error (total)	Estimated local truncation error (relative)	True local truncation error (relative)	Step-size
0.0228	9.99479$E-01$	3.2$E-14$	1.37$E-14$	1.06$E-14$	4.768$E-03$
0.7540	6.37575$E-01$	$-5.1E-09$	$-8.64E-09$	$-7.84E-09$	4.441$E-02$
2.0418	1.93461$E-01$	$-1.2E-07$	$-3.60E-09$	$-3.35E-09$	4.441$E-02$
4.0069	5.86328$E-02$	$-6.5E-08$	$-7.74E-10$	$-7.33E-10$	5.551$E-02$
7.4642	1.76322$E-02$	$-4.0E-08$	$-1.22E-09$	$-1.15E-09$	1.084$E-01$
13.0885	5.80353$E-03$	$-3.3E-08$	$-7.17E-10$	$-6.79E-10$	1.694$E-01$
18.6683	2.86117$E-03$	$-3.1E-08$	$-1.16E-09$	$-1.09E-09$	2.647$E-01$
25.3520	1.55347$E-03$	$-3.1E-08$	$-7.64E-10$	$-7.23E-10$	3.309$E-01$
40.7168	6.02823$E-04$	$-3.0E-08$	$-6.67E-10$	$-6.32E-10$	5.170$E-01$

[a] The notation $E-5$ denotes 10^{-5}.

In Table I we have the information for problem (6.1) which has a well-behaved solution (i.e., small changes in the data yield only small variations in the solution. Additionally there are no rapid oscillations or sudden changes in the slope.) No upper limit was put on the step-size, though in practice, this may be necessary. The step-size (truncation errors) listed in Table I is the one used (made) in arriving at the x-value which is printed on the same line.

The initial value problem (6.2) has a rapidly oscillating solution which grows in absolute value like e^{5x}. Calculations are given between $x = 0$ and $x = 1$ which covers 10 periods of the sine wave oscillation. Values in Table II are given in groups of successive steps to illustrate the estimates during truncation error sign changes, changes in step-sizes, and rapid changes in slope. The slope information is important, since the estimate for the local truncation error is just a linear combination of values of y and slopes.

TABLE II

x	y (calculated solution)	Relative error (total)	Slope	Estimated local truncation error (relative)	True local truncation error (relative)	Step-size
0.0255	$1.1353E+00$	$-1.09E-08$	$3.58E+00$	$-4.8E-10$	$-4.0E-10$	$1.95E-03$
0.0274	$1.1337E+00$	$-1.02E-08$	$-5.26E+00$	$1.0E-10$	$7.9E-10$	$1.95E-03$
0.0298	$1.1073E+00$	$-3.88E-09$	$-1.64E+01$	$5.9E-09$	$6.7E-09$	$2.44E-03$
0.1415	$1.0304E+00$	$1.39E-07$	$-1.05E+02$	$5.0E-08$	$3.7E-08$	$2.33E-03$
0.1427	$9.0517E-01$	$1.61E-07$	$-1.10E+02$	$2.6E-09$	$1.4E-09$	$1.16E-03$
0.1439	$7.7356E-01$	$1.91E-07$	$-1.16E+02$	$2.1E-09$	$1.7E-09$	$1.16E-03$
0.7755	$-4.8279E+01$	$1.00E-07$	$-1.47E+02$	$2.8E-10$	$2.4E-10$	$1.81E-03$
0.7773	$-4.8230E+01$	$1.01E-07$	$2.01E+02$	$-6.6E-10$	$-5.2E-10$	$1.81E-03$
0.7796	$-4.7277E+01$	$9.94E-08$	$6.41E+02$	$-3.6E-09$	$-4.3E-09$	$2.26E-03$
0.9567	$-4.9051E+01$	$1.31E-07$	$-7.09E+03$	$6.1E-10$	$7.0E-10$	$9.82E-04$
0.9577	$-5.5952E+01$	$1.16E-07$	$-6.96E+03$	$5.4E-10$	$6.0E-10$	$9.82E-04$

Small perturbations of the data in problem (6.3) cause large changes in the solution and one should, therefore, expect a scheme which progresses step by step to give very poor results. This behavior is certainly illustrated in Table III. The procedure produces step-sizes to achieve local truncation errors (relative) between the preset $T_{\max} = 5 \times 10^{-8}$ and $T_{\min} = 5 \times 10^{-10}$ despite the fact that the calculated solution diverges rapidly from the true solution. Examples like (6.3) and Table III illustrate the care which must be exercised when using any method of step-size control based on local truncation error estimation.

TABLE III

x	y (calculated solution)	Relative error (total)	Estimated local truncation error (relative)	True local truncation error (relative)	Step-size
0.0288	$3.88E-02$	$1.6E-11$	$3.6E-13$	$6.1E-13$	$7.45E-03$
0.1908	$2.01E-01$	$2.8E-05$	$-1.8E-08$	$-2.3E-08$	$7.11E-03$
0.2743	$2.61E-01$	$8.3E-02$	$-3.7E-09$	$-3.9E-09$	$8.88E-04$
0.3150	$-1.05E+00$	$4.2E+00$	$-5.0E-10$	$-5.3E-10$	$3.47E-04$
0.401	$-7.55E+03$	$1.8E+04$	$-1.2E-09$	$-1.2E-09$	$4.34E-04$
0.671	$-4.09E+15$	$6.0E+15$	$-1.2E-09$	$-1.2E-09$	$4.34E-04$
0.998	$-6.50E+29$	$6.5E+29$	$-1.2E-09$	$-1.2E-09$	$4.34E-04$

7. Conclusions

On the basis of fairly extensive numerical testing, it has been concluded that the estimate (5.1) generally yields the true local truncation error within a factor of two, which is sufficient for controlling step-size. If one wishes to keep the true local truncation error below 10^{-A}, I have found that $T_{\max} = 0.3 \times 10^{-A}$ will always suffice, though perhaps this is too conservative.

Let us relabel the τ of (5.1) as $\tau(n-1)$. Our use of $\tau(n-1)$ to control stepsize leads to disposal of values calculated at x_n and x_{n+1} if the magnitude of $\tau(n-1)$ is not acceptable. If $\tau(n-1)$ is calculated by (5.1) and then the first order approximation $\bar{\tau}(n) = \tau(n-1) + (\tau(n-1) - \tau(n-2))$ is calculated for $\tau(n)$, we always obtain at least one significant figure of agreement between the calculated $\tau(n)$ (i.e., the estimate of $\tau(n-1)$ at the next step) and $\bar{\tau}(n)$. Using $\bar{\tau}(n)$ to control step-size allows disposal of only the values at x_{n+1} in changing step-size. This works well in practice, even when there are sharp changes in the solution (we recorded changes in the slope of the solution curve from -5×10^3 to $+7 \times 10^2$ over one step of length $h = 0.0034$). However, I would still recommend the use of $\tau(n-1)$ if there are possibilities of discontinuities.

Comparison of these truncation error estimates and those for a generalized predictor–corrector scheme may be made by examining the data in [2].

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